Microcystin LR

101043-37-2 | DTXSID3031654

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 2.53

Global applicability domain: Outside

Local applicability domain index: 2.22e-01

Confidence level: 4.57e-01

Nearest Neighbors from the Training Set

Image not found	Image not found
N-(2-((1-(Cyclohexylmethyl)-2-(3-ethyl-2-oxo-5-oxazolidinyl)-2-hydroxyethyl)amino)-2-oxo-1-(2-thienylmethyl)ethyl)-gamma-oxo-alpha-(phenylmethyl)-4-morpholinebutanamide	N-(2-((1-(Cyclohexylmethyl)-2-(3-ethyl-2-oxo-5-oxazolidinyl)-2-hydroxyethyl)amino)-2-oxo-1-(2-thienylmethyl)ethyl)-gamma-oxo-alpha-(phenylmethyl)-4-morpholinebutanamide
Measured: 1.42	**Measured:** 1.22
Predicted: N/A	**Predicted:** N/A